

# 2,4-Dichlorobenzoic acid, 4-tolyl ester

Inchi:	InChI=1S/C14H10Cl2O2/c1-9-2-5-11(6-3-9)18-14(17)12-7-4-10(15)8-13(12)16/h2-8H,1H
InchiKey:	FZQYSSYQXKFJG-UHFFFAOYSA-N
Formula:	C14H10Cl2O2
SMILES:	Cc1ccc(OC(=O)c2ccc(Cl)cc2Cl)cc1
Mol. weight [g/mol]:	281.13
CAS:	92153-11-2

## Physical Properties

Property code	Value	Unit	Source
gf	5.15	kJ/mol	Joback Method
hf	-169.92	kJ/mol	Joback Method
hfus	30.11	kJ/mol	Joback Method
hvap	71.22	kJ/mol	Joback Method
log10ws	-5.40		Crippen Method
logp	4.521		Crippen Method
mcvol	192.520	ml/mol	McGowan Method
pc	2568.89	kPa	Joback Method
tb	739.17	K	Joback Method
tc	989.16	K	Joback Method
tf	469.94	K	Joback Method
vc	0.726	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	459.79	J/molxK	739.17	Joback Method
cpg	510.53	J/molxK	947.50	Joback Method
cpg	502.38	J/molxK	905.83	Joback Method
cpg	493.27	J/molxK	864.17	Joback Method
cpg	483.16	J/molxK	822.50	Joback Method
cpg	472.01	J/molxK	780.84	Joback Method
cpg	517.76	J/molxK	989.16	Joback Method
dvisc	0.0001294	Paxs	739.17	Joback Method
dvisc	0.0001576	Paxs	694.30	Joback Method

dvisc	0.0001972	Paxs	649.43	Joback Method
dvisc	0.0002551	Paxs	604.56	Joback Method
dvisc	0.0003439	Paxs	559.68	Joback Method
dvisc	0.0004884	Paxs	514.81	Joback Method
dvisc	0.0007416	Paxs	469.94	Joback Method

## Sources

<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C92153112&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C92153112&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>

## Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>dvisc:</b>	Dynamic viscosity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hvap:</b>	Enthalpy of vaporization at standard conditions
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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